

A Short Overview of Computational Nanoscience

Juan Meza
High Performance Computing Research
Lawrence Berkeley National Laboratory
<http://hpcrd.lbl.gov/~meza>

June 4, 2007

Abstract

Computational science and mathematics have taken on an increasingly larger role in scientific research. In fact, together they are now recognized as the *third pillar* of science along with theory and experimentation. This new role is a direct consequence of an increased use of computer modeling and simulation, due to the tremendous growth in computational power. Equally important, this new role is a result of a better understanding of the underlying theory and the development of new mathematical algorithms. In this talk, I'll give examples from the computational nanoscience projects at LBL and describe the role that theory, modeling, and simulation play in guiding experiments, and in understanding and predicting new phenomena.